Deformation of anisotropic Fermi surfaces due to electron-electron interactions.

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Abstract. – We analyze the deformations of the Fermi surface induced by electron-electron interactions in anisotropic two dimensional systems. We use perturbation theory to treat, on the same footing, the regular and singular regions of the Fermi surface. It is shown that, even for weak local coupling, the self-energy presents a nontrivial behavior showing momentum dependence and interplay with the Fermi surface shape. Our scheme gives simple analytical expressions based on local features of the Fermi surface.

Introduction. – An open question in the study of the interactions in anisotropic metallic systems is the deformation of the Fermi surface induced by the interactions. The Fermi surface is one of the key features needed to understand the physical properties of a material. Recent improvements in experimental resolution have led to high precision measurements of the Fermi surface (FS), and also to the determination of the many-body effects in the spectral function, as reported by ARPES experiments [1]. The interpretation of experiments in anisotropic strongly correlated systems remains a complex task [2].

The FS depends on the self-energy corrections to the quasiparticle energies, which, in turn, depend on the shape of the Fermi surface. Hence, there is an interplay between the self-energy corrections and the FS topology. For weak local interactions, the leading corrections to the FS arise from second order diagrams. The self energy, within this approximation, can show a significant momentum dependence when the initial FS is anisotropic and lies near hot spots (see below). This simultaneous calculation of the FS and the second order self energy corrections is a formidable task. Many approaches have been used to study this problem like pertubation theory [3], bosonization methods [4, 5], or perturbative Renormalization Group calculations [6–8], and the cellular dynamical mean-field theory (CDMFT), an extension of Dynamical Mean Field Theory [9].

In this work, we calculate perturbation theory corrections and use Renormalization Group arguments [10, 11] in order to study analytically the qualitative corrections to the shape of the FS induced by the electron-electron interaction. This method allows us to classify the different features of the FS from the dependence of the self-energy corrections on the value of

a high energy cutoff, Λ, defined at the beginning of the Renormalization process. As it will be shown later, one can also analyze the effects of variations in the Fermi velocity and the curvature of the non interacting FS on the self-energy corrections.

We will study two dimensional Fermi surfaces, and we will consider mostly the $t-t'$ Hubbard model, although the calculations do not depend on the microscopic model which gives rise to a particular Fermi surface. We define the model in the next section. Then, we describe the way the corrections induced by different features of the FS depend on the high energy cutoff Λ. Next, we present a detailed calculation of the changes expected for a regular FS, and make contact with results from ARPES experiments on cuprates. At the end we highlight the most relevant aspects of our calculation, and compare them with results obtained using alternative schemes.

The model. – The hamiltonian of the $t-t'$ Hubbard model is:

$$\mathcal{H}=t\sum_{s;i,j\ \mathrm{n.n.}} c^{\dagger}_{s,i}c_{s,j}+t'\sum_{s;i,j\ \mathrm{n.n.n.}} c^{\dagger}_{s,i}c_{s,j}+U\sum_{i} n_{i\uparrow}n_{i\downarrow} \tag{1}$$

where $c_{s,i}(c^{\dagger}_{s,i})$ are destruction (creation) operators for electrons of spin s on site i, $n_{i,s}=c^{\dagger}_{s,i}c_{s,i}$ is the number operator, U is the on-site repulsion, and t and t' are the nearest and next-nearest neighbors hopping amplitudes, respectively. The Fermi surfaces of the non interacting systems are defined by:

$$\epsilon_{\mathrm{F}}=\varepsilon(\vec{\mathbf{k}})=2t\left[\cos(k_x a)+\cos(k_y a)\right]+4t'\cos(k_x a)\cos(k_y a) \tag{2}$$

where a is the lattice constant (see Fig.[1]).

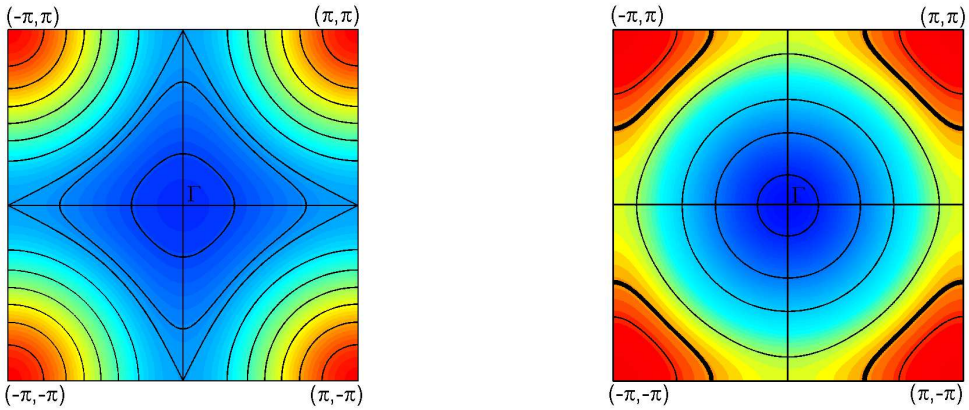

Fig. 1 – Qualitative picture of the evolution of the FS with filling from almost isotropic to convex, going through a FS exhibiting inflexion points, and one with van Hove singularities (left panel, $t'=-0.3t$). A region with almost perfect nesting is shown in the right panel ($t'=0.3t$).

Assuming that $t<0, t'>0$ and $|2t'|<|t|$, the Fermi surface is convex for $-2t+4t'\leq\epsilon_{\mathrm{F}}\leq\epsilon_0=-8t'+16t'^3/t^2$. For $-8t'+16t'^3/t^2\leq\epsilon_{\mathrm{F}}\leq-4t'$ the Fermi surface shows eight inflection points, which begin at $k_x=k_y=k_0=a^{-1}\cos^{-1}(-2t'/t)$ and move symmetrically around the $(\pm1,\pm1)$ directions, towards the center of the edges of the square Brillouin zone, $(0,\pm\pi),(\pm\pi,0)$. For $\epsilon_{\mathrm{F}}=4t'$ the Fermi surface passes through the saddle points (van Hove singularities) located at these special points of the Brillouin zone. For $4t'<\epsilon_{\mathrm{F}}\leq-4t$, the

Fermi surface is convex and hole like, centered at the corners of the Brillouin Zone, $(\pm\pi, \pm\pi)$ (See Fig.[1]). Finally, when $t' = 0$, the model has particle hole symmetry, and the Fermi surface shows perfect nesting for $\epsilon_{\rm F} = 0$.

The effects of the Hubbard interaction when the Fermi surface is near perfect nesting [12–16] or near a Van Hove singularity [17–24] have been extensively studied. Anomalous effects are also expected when the Fermi surface has inflection points [25, 26].

Self-energy corrections to singular Fermi surfaces. – The corrections to the non interacting Fermi surface are given by the real part of the self energy. Using second order perturbation theory, the self energy is given by the diagrams shown in Fig.[2]. In the following, we assume that the effect of the high energy electron-hole pairs on the quasiparticles near the Fermi surface have been integrated out, leading to a renormalization of the parameters t, t' and U of the hamiltonian, neglecting the possibility that other couplings are generated. Thus, the hamiltonian, eq.(1), describes low temperature processes below a high energy cutoff, $\Lambda \ll t, t'$. For consistency, $U \leq \Lambda$. We also assume that the Fermi surface of the interacting system exists, and that it has the same topology as that of the non interacting system.

The frequency dependence of the imaginary part of the self energy in a nested region of the Fermi surface, or at van Hove singularities is known to be linear, unlike the usual quadratic dependence expected in Landau's theory of a Fermi liquid.

$$\mathrm{Im}\Sigma_2(\vec{\mathbf{k}}, \epsilon_{\vec{\mathbf{k}}}) \propto |\epsilon_{\vec{\mathbf{k}}}| \tag{3}$$

where $\epsilon_{\vec{\mathbf{k}}} = \varepsilon(\vec{\mathbf{k}}) - \epsilon_{\rm F}$. Away from the hot spots, the leading contribution to the two loop self energy, when the Fermi surface is near a van Hove singularity, comes from diagrams where the polarizability bubble, $\Pi(\vec{\mathbf{q}}, \omega)$, involves transitions near the saddle point [27]. Near a nesting situation, the polarizability at low momenta is similar to that of a one dimensional Fermi liquid. The susceptibilities can be written as:

$$\Pi(\vec{\mathbf{q}}, \omega) \sim \begin{cases} W^{-1} \tilde{\Pi}_{\rm vH} \left(\frac{\omega}{m^* |\vec{\mathbf{q}}|^2} \right) & \text{van Hove} \\ W^{-1} \tilde{\Pi}_{\rm 1D} \left(\frac{\omega}{v_{\rm F} |\vec{\mathbf{q}}|} \right) & \text{nesting} \end{cases} \tag{4}$$

where $v_{\rm F}$ is the normal Fermi velocity in the nesting situation, and m^* is an average of the second derivative of the bands at the saddle point. Note that, in both cases, the density of states is proportional to $W^{-1} \sim t^{-1}, t'^{-1}$.

The imaginary part of the second order self energy near the regular regions of the Fermi surface can be written as [27]:

$$\mathrm{Im}\Sigma_2(\vec{\mathbf{k}}, \epsilon_{\vec{\mathbf{k}}}) \sim \int_0^{\epsilon_{\vec{\mathbf{k}}}} d\omega \int_0^{q_{\rm max}} dq \, \mathrm{Im}\Pi(q, \omega) \tag{5}$$

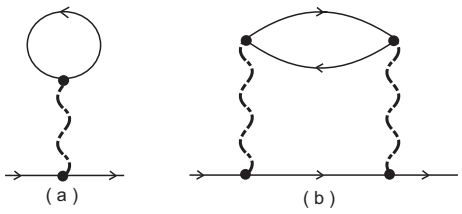

Fig. 2 – Low order self energy diagrams. Left: Hartree diagram. Right: two loop correction.

where $q_{\max} \sim |\Lambda|/v_{\rm F}$, and $v_{\rm F}$ is the Fermi velocity in these regions. Using eq.(4), we find:

$$\mathrm{Im}\Sigma_2(\vec{\mathbf{k}}, \epsilon_{\vec{\mathbf{k}}}) \propto \begin{cases} \epsilon_{\vec{\mathbf{k}}}^{3/2} & \text{van Hove} \\ \epsilon_{\vec{\mathbf{k}}}^{2} & \text{nesting} \end{cases} \tag{6}$$

We recover the usual Fermi liquid result for the regular parts of the Fermi surface near almost nested regions. This result arises from the fact that the small momentum response of a quasi–one–dimensional metal does not differ qualitatively from that predicted by Landau's theory of a Fermi liquid.

Finally, near an inflection point, we can use the techniques developed in [25,26] to obtain:

$$\mathrm{Im}\Sigma_2(\vec{\mathbf{k}}, \epsilon_{\vec{\mathbf{k}}}) \propto \epsilon_{\vec{\mathbf{k}}}^{3/2} \tag{7}$$

It is finally worth noting that there is another special point, where the Fermi surface changes from convex to concave and a pair of inflection points are generated for $\epsilon_{\rm F} = \epsilon_0$ and $\vec{\mathbf{k}} \equiv (k_0, k_0)$ defined earlier. At this point, the imaginary part of the self energy behaves as $\mathrm{Im}\Sigma_2(\vec{\mathbf{k}}, \epsilon_{\vec{\mathbf{k}}}) \propto \epsilon_{\vec{\mathbf{k}}}^{5/4}$.

We can obtain the real part of the self energy from the imaginary part by a Kramers-Kronig transformation, and restricting the frequency integral to the interval $0 \leq \omega \leq \Lambda$. We obtain:

$$\mathrm{Re}\Sigma_2(\vec{\mathbf{k}}, \epsilon_{\vec{\mathbf{k}}}) \propto -g^2|\Lambda| \times \begin{cases} \log^2\left(\frac{\Lambda}{\epsilon_{\vec{\mathbf{k}}}}\right) & \text{van Hove} \\ \log\left(\frac{\Lambda}{\epsilon_{\vec{\mathbf{k}}}}\right) & \text{nesting} \end{cases} \tag{8}$$

where the negative sign is due to the fact that it is a second order contribution in perturbation theory, and g is a dimensionless coupling constant of order U/W. The sign is independent of the sign of U in eq.(1). In the regular parts of the Fermi surface, eq.(6) leads to:

$$\mathrm{Re}(\vec{\mathbf{k}}, \epsilon_{\vec{\mathbf{k}}}) \propto \begin{cases} -g^2 \frac{|\Lambda|^{3/2}}{W^{1/2}} & \text{van Hove} \\ -g^2 \frac{|\Lambda|^2}{W} & \text{nesting} \end{cases} \tag{9}$$

where the additional powers in W arise from the m^* and $v_{\rm F}$ factors in the susceptibility, eq.(4).

In the limit $\Lambda/W \to 0$, the different dependence on Λ of the self-energy corrections at different regions of the Fermi surface is enough to give a qualitative description of the changes of the Fermi surface. For instance, when the non interacting Fermi surface is close to the saddle point, $\vec{\mathbf{k}} \equiv a^{-1}(\pm\pi, 0), a^{-1}(0, \pm\pi)$, the self-energy correction is negative and highest in this region. Note that the logarithmic divergences in eq.(8) are regularized by the temperature or elastic scattering.

In order to remove the Fermi surface from a van Hove point or nesting situation, a large number of electrons must be added to the regular regions. When the points of the FS near these hot spots are at distance k from the hot spot, the change in the self energy needed to shift the Fermi momentum by an amount δk is, using eq.(8), $\delta\Sigma \propto g^2\Lambda\frac{\delta k}{k}$ with additional logarithmic corrections near a van Hove singularity. Near the regular regions of the Fermi surface, a shift in energy of order $\delta\Sigma$ leads to a change in the momentum normal to the Fermi surface of magnitude $\delta k_{\rm reg} \sim \delta\Sigma/v_{\rm F}$. The area covered in this shift gives the number of electrons which are added to the system near the regular regions of the Fermi surface. We find $\delta n \sim k_{\max}\delta k_{\rm reg} \sim g^2 \frac{k_{\max}\Lambda}{v_{\rm F}} \frac{\delta k}{k}$ where $k_{\max} \sim a^{-1}$ determines the size of the regular regions of the Fermi surface. The value of δn diverges as the Fermi surface moves towards the hot spot, $k \to 0$. Hence, the number of electrons needed to shift the FS away from the hot spot also diverges. This analysis essentially reproduces the calculation at fixed chemical potential in the presence of a reservoir with regular self-energy corrections given in [24, 28] (a different analysis [29] does not make use of a reservoir).

Self-energy corrections to regular Fermi surfaces. – We study now the system at a filling which yields a curved FS, slightly anisotropic, in the absence of singularities. Near the Fermi surface the electronic dispersion can be approximated by:

$$\epsilon_{\vec{\mathbf{k}}} = v_F \kappa_\perp + \beta \kappa_\parallel^2 \tag{10}$$

where $\kappa_\parallel$ is the momentum parallel to the FS, $\kappa_\parallel = (\vec{\mathbf{k}} - \vec{\mathbf{k}}_F)_\parallel$, $\kappa_\perp$ is the momentum perpendicular to the FS relative to k_F, $\kappa_\perp = (\vec{\mathbf{k}} - \vec{\mathbf{k}}_F)_\perp$, v_F is the Fermi velocity $v_F = \hat{\mathbf{n}}_\perp \cdot \nabla \varepsilon(\vec{\mathbf{k}})$ and β is related to the local curvature of the Fermi surface $b = \hat{\mathbf{n}}_\parallel \cdot \left(\nabla^2 \varepsilon(\vec{\mathbf{k}}) \right) \hat{\mathbf{n}}_\parallel$, by $\beta = b v_F/2$. The Fermi velocity v_F and the FS curvature b, are functions of $t, t', \epsilon_{\mathrm{F}}$ and the position along the Fermi line. We assume that the main contribution to the self energy arises from processes where the momentum transfer is small, or from processes which involve scattering from the region under consideration to the opposite part of the Fermi surface, *i. e.*, backward scattering. This assumption can be justified by noting that the Hubbard interaction is momentum independent, so that the leading effects are associated to the structure of the density of states. The processes discussed here have the highest joint density of states.

Using the parametrization in eq.(10), the imaginary part of the self energy, which describes the decay of quasiparticles in the region under consideration, is independent of the cutoff Λ. The contribution from forward scattering processes is:

$$Im\Sigma_2(\vec{\mathbf{k}}, \omega) = \frac{3}{64} \frac{U^2 a^4}{\sqrt{2}\pi^2} \frac{\omega^2}{v_F^2 |\beta|} \ . \tag{11}$$

The quadratic dependence of energy is expected, and consistent with Landau's theory of a Fermi liquid. This contribution diverges as $v_{\mathrm{F}} \to 0$, that is, when the Fermi surface approaches a van Hove singularity, or as $|b| \to 0$ which signals the presence of an inflection point or nesting. The contribution due to backward scattering is exactly the same as that from forward scattering, eq.(11), with the same numerical prefactors.

Using a Kramers-Kronig transformation, and integrating again in the interval $0 \leq \omega \leq \Lambda$, we obtain:

$$Re\Sigma_2(\vec{\mathbf{k}}, \omega = 0) = -\frac{3}{64} \frac{U^2 a^4}{\sqrt{2}\pi^3} \frac{\Lambda^2}{v_F^2 |\beta|} \tag{12}$$

This expression gives the leading corrections to the shape of the FS. Notice that both, v_{F} and β, are momentum dependent.

In Fig.[3](a)-(b), the bare (thin black line) and renormalized (thick red line) Fermi surfaces are shown at two different densities in the first quadrant of the Brillouin zone (BZ) for the parameter values $t = -1$, $t' = -0.3t$, reminiscent of hole-doped cuprates. At the density shown in Fig.[3](a) the self-energy corrections are stronger in the less curved regions of the FS around the diagonal parts of the BZ. This correction coincides with that found in [30] for the renormalization of a flat FS by a two-loop field theory RG approach, where interactions induce a small curvature to the bare flat FS. When we change the filling, the FS shape varies, and close to half-filling the FS has the form shown in Fig.[3](b). The change in shape qualitatively agrees with the doping evolution of k_F measured by ARPES on cuprates [31, 32]. The self energy corrections, close to half-filling, enhance the hole-like curvature and flatten the FS close to the $(\pi, 0)$ and $(0, \pi)$ points of the BZ as shown in Fig.[3](b).

In Fig.[3](c) we show the FS corresponding to $t = -1, t' = 0.3t$ $(t/t' > 0)$ reminiscent of the electron-doped cuprates, close to half-filling, at a similar density as the one represented in Fig.[3](b). The self-energy corrections here are stronger at the most curved regions of the

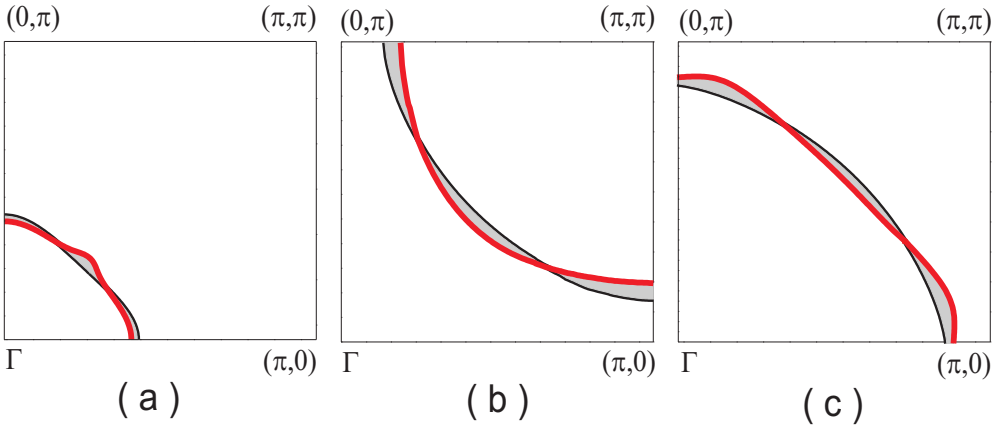

Fig. 3 – Deformations induced by the interactions on the FS of the $t-t'$ Hubbard model, in the first quadrant of the Brillouin zone. Thin black line represents the unperturbed FS while the thick red line represents the FS corrected by the interaction, the shadowed region corresponds to their difference. For $t'/t = -0.3$ (a): high doping range and (b) close to half filling. For $t'/t = +0.3$ (c)close to half filling.

FS, in the proximity of the saddle points (where v_F diverges). The corrected FS is closer to a nesting situation than the bare FS. Our results, near half-filling, are in overall agreement with those of [9], although we find that the self energy corrections are stronger at the antinodal region in both hole-like and electron-like Fermi surfaces.

Conclusions. – We have presented a simplified way of taking into account the self-energy corrections to the Fermi surface. We have made use of the different dependences of the self energy on the high energy cutoff in order to analyze the main features of the changes of the FS. The results suggest that the main self-energy corrections, which are always negative, peak when the FS is close to the $(\pm\pi, 0), (0, \pm\pi)$ points in the Brillouin zone. If these contributions are cast as corrections to the hopping elements of the initial hamiltonian, we find that the nearest neighbor hopping, t, is weakly changed (as it does not contribute to the band dispersion in these regions). The next nearest neighbor hopping, t' which shifts the bands by $-4t'$ in this region, acquires a negative correction. This implies that the absolute value of t' grows when $t' > 0$, or decreases, when $t' < 0$, in reasonable agreement with the results in [9]. Note that the tendency observed in our calculation towards the formation of flat regions near these points, when analyzed in higher order perturbation theory, will lead to stronger corrections. Our results also confirm the pinning of the FS near saddle points, due to the interactions. The analysis is consistent with the measured Fermi surfaces of the cuprates [1] and qualitatively agree with the doping evolution reported by ARPES [1, 31, 32].

Finally the analysis presented here is valid only at weak coupling, and we do not consider corrections to the interactions or to the wave-function renormalization. The main goal of this scheme is that can be used with different models and the expressions obtained are analytical and related to the local features of the non-interacting FS in a simple way, so that they can be readily used to get an estimate of the corrections expected.

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